# Theory and simulations of crystalline control via salinity and pH in ionizable membranes

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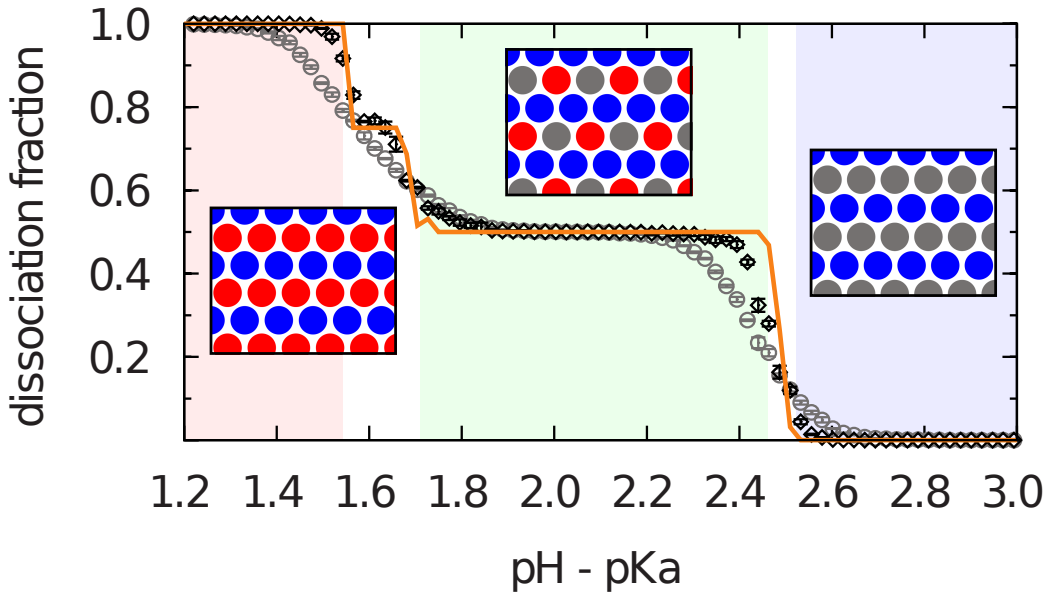
We study a dense two-dimensional binary mixture consisting of ionized amphiphiles with equal concentrations of positive and negative species. We analyze this co-assembled system by numerically exact optimization and by continuum Monte Carlo simulations including short range and electrostatic interactions among all the particles. We find the optimal structure to be a triangular lattice for high salt concentrations, a face-centered rectangular lattice for intermediate salt concentrations, and a square lattice for low salt concentrations. At neutral pH, this crossover occurs gradually over a wide range of salt concentrations, while for highly acidic or basic solutions, it is much more abrupt. At intermediate values of pH, the unit cells become more complicated, causing the dissociation curve to follow a staircase function.




*Simulation results showing dissociation as a function of pH. The insets correspond to the stable lattice structures seen for the plateaus of the plot, with blue circles being positive ions, red being negative, and gray being neutral.*

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